Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 03:01 PM EDT

PDB ID	:	1SZG
Title	:	A198G:L230A flavocytochrome b2 with sulfite bound
Authors	:	Mowat, C.G.; Wehenkel, A.; Green, A.J.; Walkinshaw, M.D.; Reid, G.A.; Chapman, S.K.
Deposited on	:	2004-04-05
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

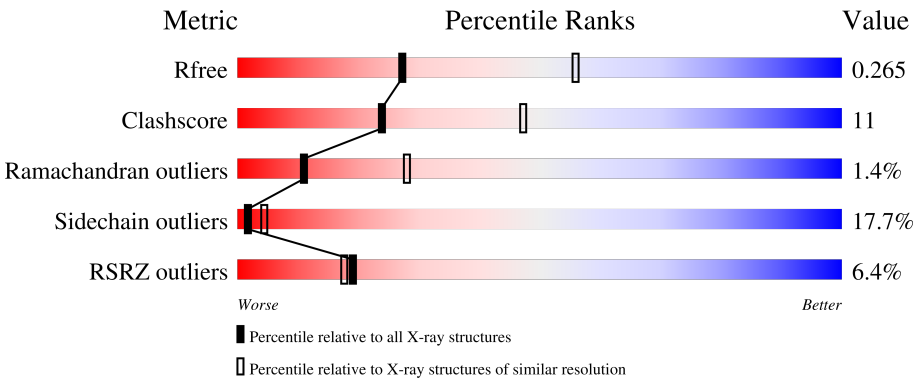
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	511	4% 53% 19% • • 23%
1	B	511	6% 50% 20% 6% 24%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FNS	B	9570	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6255 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

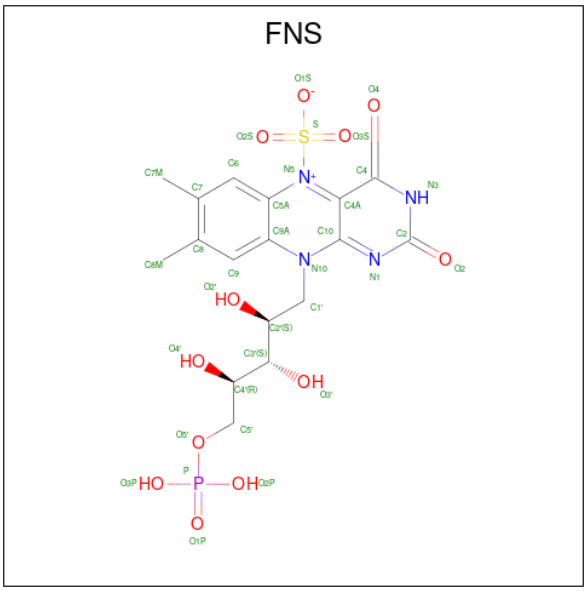
- Molecule 1 is a protein called Cytochrome b2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	392	3040	1927	518	584	11	0	0	1
1	B	387	3014	1911	513	579	11	0	0	1

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	GLY	ALA	engineered mutation	UNP P00175
A	230	ALA	LEU	engineered mutation	UNP P00175
B	198	GLY	ALA	engineered mutation	UNP P00175
B	230	ALA	LEU	engineered mutation	UNP P00175

- Molecule 2 is N-SULFO-FLAVIN MONONUCLEOTIDE (three-letter code: FNS) (formula: $C_{17}H_{21}N_4O_{12}PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	35	17	4	12	1	1	0	0
			Total	C	N	O	P	S		
2	B	1	35	17	4	12	1	1	0	0

- Molecule 3 is water.

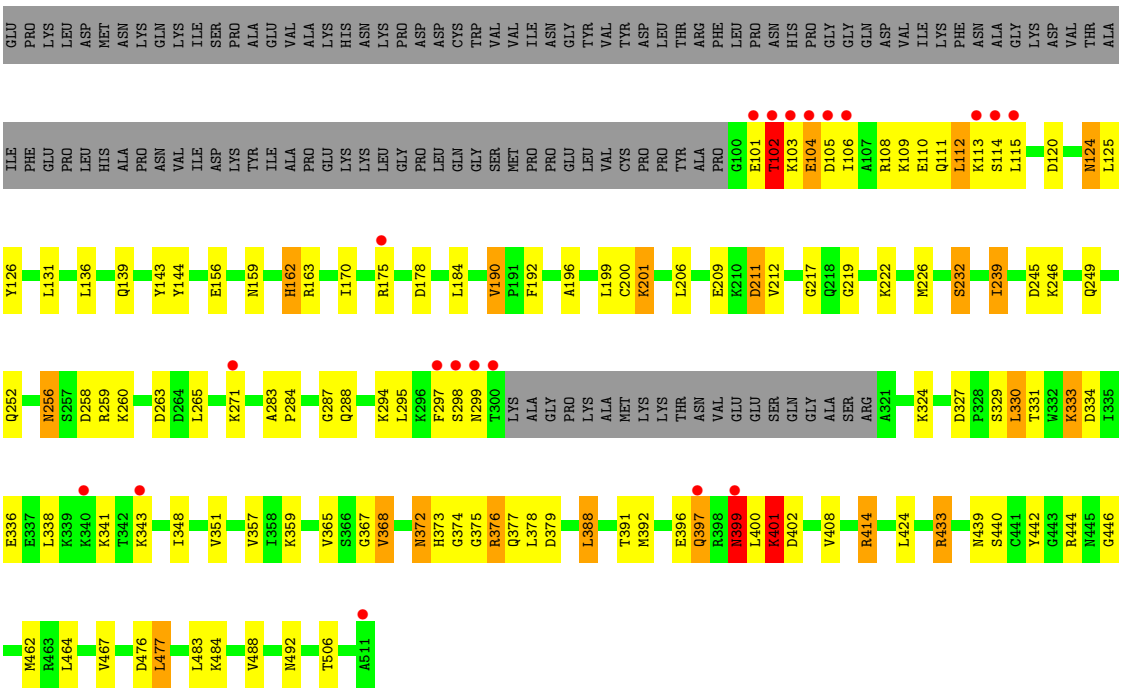
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	78	78	78	0	0
			Total	O		
3	B	53	53	53	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

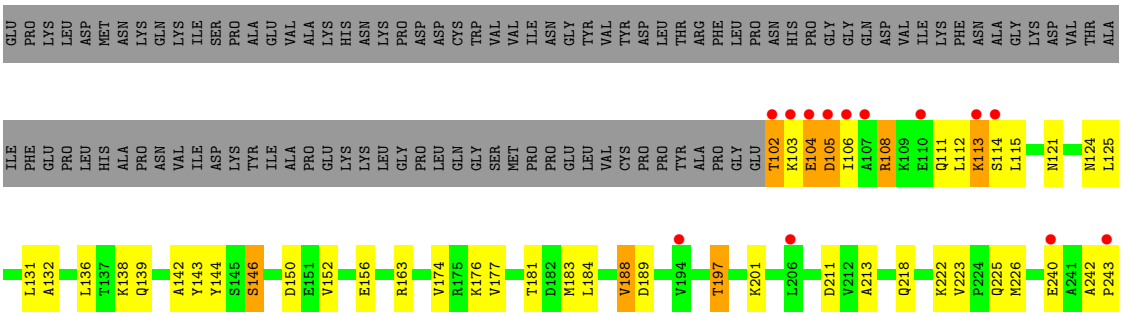
• Molecule 1: Cytochrome b2, mitochondrial

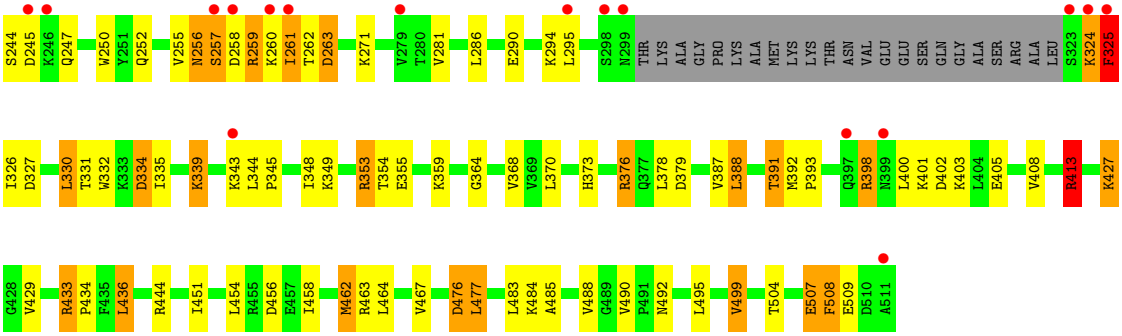
Chain A:



• Molecule 1: Cytochrome b2, mitochondrial

Chain B:




S244 D245 K246 Q247 W250 Y251 Q252 V255 N256 S257 D258 R259 K260 I261 T262 D263 K271 V279 T280 V281 L286 E290 K294 L295 S298 N299 THR LYS ALA GLY PRO LYS ALA MET LYS LYS THR ASN VAL GLU GLU SER GLN GLY ALA SER ARG ALA LEU S323 K324 F325
I326 D327 L330 T331 W332 K333 D334 I335 K339 K343 L344 P345 I348 K349 R353 T354 E355 K359 G364 V368 V369 L370 H373 R376 Q377 L378 D379 V387 L388 T391 M392 P393 Q397 R398 M399 L400 K401 D402 K403 L404 E405 V408 R413 K427
G428 V429 R433 P434 F435 L436 R444 I451 L454 R455 D456 E457 I458 M462 R463 L464 V467 D476 L477 L483 K484 A485 V488 G489 V490 P491 N492 L495 V499 T504 E507 F508 E509 D510 A511

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	163.97Å 163.97Å 112.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.00 – 2.70 23.89 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.0 (24.00-2.70) 91.0 (23.89-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.223 , 0.266 0.224 , 0.265	Depositor DCC
R_{free} test set	2233 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 68.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6255	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FNS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.53	0/3089	0.87	10/4172 (0.2%)
1	B	0.59	6/3063 (0.2%)	0.86	12/4138 (0.3%)
All	All	0.56	6/6152 (0.1%)	0.86	22/8310 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	GLU	CD-OE2	6.91	1.33	1.25
1	B	240	GLU	CD-OE1	6.04	1.32	1.25
1	B	104	GLU	CD-OE1	5.71	1.31	1.25
1	B	325	PHE	CE2-CZ	5.53	1.47	1.37
1	B	325	PHE	CE1-CZ	5.34	1.47	1.37
1	B	325	PHE	CD1-CE1	5.01	1.49	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	112	LEU	CA-CB-CG	6.64	130.56	115.30
1	A	211	ASP	CB-CG-OD2	6.49	124.14	118.30
1	B	413	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	376	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	189	ASP	CB-CG-OD2	5.78	123.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	120	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	376	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	263	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	413	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	263	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	402	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	379	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	433	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	B	334	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	476	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	211	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	245	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	433	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	245	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	379	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	178	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	456	ASP	CB-CG-OD2	5.02	122.82	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	492	ASN	CA

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3040	0	3090	56	0
1	B	3014	0	3067	81	0
2	A	35	0	19	2	0
2	B	35	0	19	11	0
3	A	78	0	0	5	0
3	B	53	0	0	1	0
All	All	6255	0	6195	137	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:TYR:O	1:B:376:ARG:NH2	2.00	0.94
1:A:143:TYR:O	1:A:376:ARG:NH2	2.01	0.94
1:B:197:THR:HG21	1:B:436:LEU:HG	1.46	0.93
1:B:413:ARG:HH22	2:B:9570:FNS:P	1.98	0.86
1:B:183:MET:CE	1:B:250:TRP:HH2	1.93	0.79
1:B:243:PRO:HD2	1:B:247:GLN:HE22	1.46	0.79
1:B:105:ASP:HA	1:B:108:ARG:HB2	1.64	0.79
1:A:331:THR:HG22	1:A:333:LYS:H	1.54	0.72
1:B:507:GLU:O	1:B:508:PHE:HB2	1.90	0.72
1:A:201:LYS:HB2	1:A:232:SER:OG	1.90	0.72
1:B:104:GLU:HG2	1:B:105:ASP:N	1.90	0.71
1:B:256:ASN:HD22	1:B:258:ASP:H	1.39	0.71
1:A:109:LYS:O	1:A:113:LYS:HB2	1.92	0.70
1:A:367:GLY:O	3:A:5645:HOH:O	2.09	0.69
1:A:136:LEU:HD21	1:A:440:SER:HB3	1.73	0.69
1:A:414:ARG:HD2	1:B:150:ASP:OD2	1.92	0.69
1:A:196:ALA:HB2	1:A:226:MET:HE2	1.75	0.69
1:A:256:ASN:HD22	1:A:258:ASP:H	1.43	0.66
1:B:388:LEU:HD22	1:B:392:MET:HG2	1.77	0.66
1:A:373:HIS:O	1:A:376:ARG:HG3	1.96	0.65
1:B:142:ALA:O	1:B:146:SER:HB2	1.97	0.65
2:B:9570:FNS:O4'	2:B:9570:FNS:H9	1.97	0.65
1:B:433:ARG:HG3	2:B:9570:FNS:C8M	2.27	0.65
1:B:223:VAL:HG21	1:B:451:ILE:HG12	1.81	0.63
1:B:339:LYS:HE3	1:B:364:GLY:O	1.99	0.63
1:A:219:GLY:O	1:A:222:LYS:NZ	2.32	0.62
1:B:325:PHE:HB3	1:B:326:ILE:HG13	1.79	0.62
1:B:259:ARG:NH1	1:B:327:ASP:OD2	2.32	0.62
1:B:349:LYS:CE	2:B:9570:FNS:O2	2.48	0.62
1:A:351:VAL:HG21	1:A:368:VAL:HG22	1.83	0.61
1:B:183:MET:HE2	1:B:250:TRP:HH2	1.65	0.61
1:B:434:PRO:HG3	3:B:9622:HOH:O	2.00	0.61
1:A:156:GLU:OE2	1:A:163:ARG:NH2	2.36	0.59
1:B:405:GLU:HG2	1:B:427:LYS:HD3	1.85	0.58
1:B:108:ARG:HH22	1:B:138:LYS:HG3	1.66	0.58
1:A:348:ILE:HB	3:A:5645:HOH:O	2.03	0.58
2:A:5570:FNS:H9	2:A:5570:FNS:O4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:GLU:OE2	1:B:163:ARG:NH2	2.37	0.57
1:A:372:ASN:HD22	1:A:375:GLY:H	1.53	0.56
1:B:104:GLU:OE1	1:B:108:ARG:NH1	2.40	0.55
1:B:218:GLN:HE22	1:B:444:ARG:HH11	1.54	0.55
1:B:256:ASN:HD22	1:B:258:ASP:N	2.05	0.54
1:A:124:ASN:ND2	1:A:126:TYR:HB2	2.23	0.54
1:B:255:VAL:HB	1:B:262:THR:HG21	1.90	0.54
1:A:259:ARG:NH1	1:A:327:ASP:OD2	2.35	0.54
1:B:256:ASN:ND2	1:B:258:ASP:H	2.06	0.54
1:A:399:ASN:C	1:A:401:LYS:H	2.11	0.53
1:B:197:THR:HG22	1:B:197:THR:O	2.09	0.53
1:B:387:VAL:O	1:B:391:THR:HG23	2.08	0.53
1:B:454:LEU:O	1:B:458:ILE:HG13	2.08	0.53
1:A:399:ASN:O	1:A:401:LYS:N	2.42	0.53
1:B:259:ARG:NH2	1:B:334:ASP:OD1	2.41	0.53
1:B:349:LYS:HE2	2:B:9570:FNS:O2	2.09	0.53
1:B:104:GLU:CG	1:B:105:ASP:N	2.68	0.52
1:B:121:ASN:HD22	1:B:121:ASN:N	2.07	0.52
1:B:156:GLU:CD	1:B:163:ARG:HH22	2.13	0.52
1:A:196:ALA:CB	1:A:226:MET:HE2	2.40	0.52
1:B:413:ARG:NH2	2:B:9570:FNS:P	2.77	0.52
1:B:144:TYR:O	1:B:433:ARG:HD3	2.10	0.52
1:B:183:MET:HE2	1:B:250:TRP:CH2	2.45	0.51
1:A:190:VAL:HG13	1:A:192:PHE:H	1.75	0.51
1:A:372:ASN:ND2	1:A:375:GLY:H	2.09	0.50
1:B:183:MET:CE	1:B:250:TRP:CH2	2.85	0.50
1:B:132:ALA:O	1:B:136:LEU:HG	2.12	0.50
1:A:259:ARG:HH21	1:A:334:ASP:CG	2.15	0.49
1:A:388:LEU:HD22	1:A:392:MET:HG2	1.94	0.49
1:B:353:ARG:HG2	1:B:355:GLU:OE1	2.11	0.49
1:A:143:TYR:CZ	1:A:199:LEU:HD12	2.48	0.49
2:B:9570:FNS:C10	2:B:9570:FNS:HO2'	2.25	0.49
1:A:348:ILE:HD12	1:A:365:VAL:HG11	1.95	0.49
1:A:101:GLU:HA	1:A:104:GLU:OE1	2.13	0.48
1:B:242:ALA:HB1	1:B:247:GLN:CD	2.33	0.48
1:B:111:GLN:HA	1:B:115:LEU:HB2	1.95	0.48
1:A:467:VAL:HG11	1:A:477:LEU:HD21	1.95	0.48
1:B:113:LYS:O	1:B:115:LEU:N	2.44	0.48
1:B:177:VAL:HG13	1:B:462:MET:HE2	1.95	0.48
1:B:213:ALA:HB2	1:B:225:GLN:HE22	1.79	0.48
1:A:144:TYR:O	1:A:433:ARG:HD3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:GLY:O	1:A:433:ARG:NH2	2.39	0.47
1:B:400:LEU:HD23	1:B:403:LYS:HG3	1.95	0.47
2:B:9570:FNS:O4	2:B:9570:FNS:S	2.72	0.47
1:B:256:ASN:HD22	1:B:257:SER:N	2.13	0.47
1:A:162:HIS:HE1	3:A:5606:HOH:O	1.98	0.46
1:B:183:MET:HE3	1:B:250:TRP:HH2	1.79	0.46
1:B:174:VAL:CG2	1:B:463:ARG:HG3	2.46	0.46
1:A:388:LEU:HD13	1:A:424:LEU:HB2	1.97	0.46
1:A:211:ASP:HB3	1:A:439:ASN:HD21	1.80	0.46
1:A:239:ILE:HA	1:A:249:GLN:HE22	1.81	0.45
1:A:488:VAL:HG22	1:B:490:VAL:HG13	1.99	0.45
1:B:398:ARG:HG3	1:B:400:LEU:HD12	1.99	0.45
1:A:102:THR:HB	3:A:5642:HOH:O	2.17	0.45
1:A:159:ASN:HB3	1:B:488:VAL:HG11	1.99	0.45
1:A:414:ARG:HH11	1:B:150:ASP:CG	2.20	0.45
1:B:462:MET:HE3	1:B:467:VAL:HG23	1.97	0.45
1:B:335:ILE:HG21	1:B:348:ILE:HD11	1.98	0.44
1:B:495:LEU:O	1:B:499:VAL:HG22	2.18	0.44
1:B:104:GLU:C	1:B:106:ILE:H	2.20	0.44
1:B:104:GLU:C	1:B:106:ILE:N	2.70	0.44
1:B:163:ARG:HD2	1:B:485:ALA:O	2.16	0.44
1:A:124:ASN:HD21	1:A:126:TYR:HB2	1.81	0.44
1:B:242:ALA:HB1	1:B:247:GLN:NE2	2.32	0.44
1:A:102:THR:C	1:A:104:GLU:H	2.19	0.44
1:A:113:LYS:C	1:A:115:LEU:H	2.20	0.43
1:B:467:VAL:HG11	1:B:477:LEU:HD21	2.00	0.43
1:A:399:ASN:HD22	1:A:399:ASN:HA	1.63	0.43
1:B:331:THR:HG22	1:B:332:TRP:N	2.33	0.43
2:A:5570:FNS:O2S	2:A:5570:FNS:C4	2.66	0.43
1:A:170:ILE:HG12	1:B:281:VAL:HG23	2.00	0.43
1:B:324:LYS:O	1:B:325:PHE:C	2.57	0.43
1:B:226:MET:HE2	1:B:252:GLN:HB2	2.01	0.43
1:A:287:GLY:H	1:A:377:GLN:NE2	2.17	0.42
1:B:181:THR:O	1:B:188:VAL:HG23	2.20	0.42
1:B:413:ARG:NH2	2:B:9570:FNS:O3P	2.49	0.42
1:A:442:TYR:HB2	1:A:446:GLY:HA3	2.00	0.42
1:B:255:VAL:HG13	1:B:330:LEU:HD11	2.00	0.42
1:B:392:MET:HB2	1:B:393:PRO:HD3	2.00	0.42
1:B:354:THR:HG23	1:B:391:THR:HB	2.02	0.42
1:A:163:ARG:NH1	1:B:488:VAL:O	2.53	0.42
1:B:102:THR:HB	1:B:104:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ALA:N	1:A:284:PRO:CD	2.82	0.42
1:A:484:LYS:HA	1:A:484:LYS:HD2	1.67	0.42
1:A:105:ASP:O	1:A:109:LYS:HB2	2.20	0.41
1:A:368:VAL:HG23	3:A:5645:HOH:O	2.20	0.41
1:B:398:ARG:O	1:B:400:LEU:HG	2.19	0.41
1:A:200:CYS:HB2	1:A:209:GLU:OE2	2.20	0.41
1:A:414:ARG:NH2	1:B:290:GLU:OE2	2.54	0.41
1:A:329:SER:O	1:A:330:LEU:C	2.58	0.41
2:B:9570:FNS:O4	2:B:9570:FNS:O2S	2.38	0.41
1:A:196:ALA:H	1:A:226:MET:HE1	1.85	0.41
1:B:174:VAL:HG21	1:B:463:ARG:HG3	2.03	0.41
1:B:400:LEU:HA	1:B:403:LYS:HG3	2.02	0.41
1:B:258:ASP:HB3	1:B:261:ILE:HG13	2.03	0.40
2:B:9570:FNS:O2S	2:B:9570:FNS:C4	2.68	0.40
1:B:344:LEU:HA	1:B:345:PRO:HD3	1.86	0.40
1:A:217:GLY:HA2	1:A:222:LYS:HG2	2.03	0.40
1:A:357:VAL:HG21	1:A:391:THR:HG21	2.02	0.40
1:B:387:VAL:O	1:B:391:THR:CG2	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	388/511 (76%)	364 (94%)	16 (4%)	8 (2%)	7 18
1	B	383/511 (75%)	360 (94%)	20 (5%)	3 (1%)	19 43
All	All	771/1022 (75%)	724 (94%)	36 (5%)	11 (1%)	11 28

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	LEU
1	A	299	ASN
1	A	397	GLN
1	B	105	ASP
1	B	325	PHE
1	A	298	SER
1	A	401	LYS
1	A	102	THR
1	A	114	SER
1	A	399	ASN
1	B	508	PHE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	334/439 (76%)	277 (83%)	57 (17%)	2 5
1	B	333/439 (76%)	272 (82%)	61 (18%)	1 4
All	All	667/878 (76%)	549 (82%)	118 (18%)	2 4

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	THR
1	A	103	LYS
1	A	104	GLU
1	A	106	ILE
1	A	108	ARG
1	A	110	GLU
1	A	111	GLN
1	A	112	LEU
1	A	124	ASN
1	A	125	LEU
1	A	131	LEU
1	A	139	GLN
1	A	162	HIS

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Mol	Chain	Res	Type
1	A	175	ARG
1	A	184	LEU
1	A	190	VAL
1	A	201	LYS
1	A	206	LEU
1	A	212	VAL
1	A	232	SER
1	A	239	ILE
1	A	246	LYS
1	A	252	GLN
1	A	256	ASN
1	A	260	LYS
1	A	265	LEU
1	A	271	LYS
1	A	288	GLN
1	A	294	LYS
1	A	295	LEU
1	A	297	PHE
1	A	324	LYS
1	A	330	LEU
1	A	333	LYS
1	A	336	GLU
1	A	338	LEU
1	A	341	LYS
1	A	343	LYS
1	A	359	LYS
1	A	368	VAL
1	A	372	ASN
1	A	378	LEU
1	A	388	LEU
1	A	396	GLU
1	A	397	GLN
1	A	399	ASN
1	A	401	LYS
1	A	408	VAL
1	A	414	ARG
1	A	444	ARG
1	A	462	MET
1	A	464	LEU
1	A	476	ASP
1	A	477	LEU
1	A	483	LEU

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Mol	Chain	Res	Type
1	A	492	ASN
1	A	506	THR
1	B	102	THR
1	B	103	LYS
1	B	108	ARG
1	B	112	LEU
1	B	113	LYS
1	B	114	SER
1	B	124	ASN
1	B	125	LEU
1	B	131	LEU
1	B	139	GLN
1	B	146	SER
1	B	152	VAL
1	B	176	LYS
1	B	184	LEU
1	B	188	VAL
1	B	197	THR
1	B	201	LYS
1	B	222	LYS
1	B	244	SER
1	B	256	ASN
1	B	257	SER
1	B	259	ARG
1	B	260	LYS
1	B	261	ILE
1	B	263	ASP
1	B	271	LYS
1	B	286	LEU
1	B	294	LYS
1	B	295	LEU
1	B	324	LYS
1	B	325	PHE
1	B	330	LEU
1	B	339	LYS
1	B	343	LYS
1	B	353	ARG
1	B	359	LYS
1	B	368	VAL
1	B	370	LEU
1	B	373	HIS
1	B	378	LEU

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Mol	Chain	Res	Type
1	B	388	LEU
1	B	391	THR
1	B	398	ARG
1	B	401	LYS
1	B	402	ASP
1	B	408	VAL
1	B	413	ARG
1	B	427	LYS
1	B	429	VAL
1	B	436	LEU
1	B	462	MET
1	B	464	LEU
1	B	476	ASP
1	B	477	LEU
1	B	483	LEU
1	B	484	LYS
1	B	492	ASN
1	B	499	VAL
1	B	504	THR
1	B	507	GLU
1	B	509	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	157	ASN
1	A	159	ASN
1	A	218	GLN
1	A	225	GLN
1	A	249	GLN
1	A	252	GLN
1	A	256	ASN
1	A	268	ASN
1	A	288	GLN
1	A	372	ASN
1	A	377	GLN
1	A	397	GLN
1	A	399	ASN
1	A	439	ASN
1	A	497	ASN
1	B	121	ASN

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Mol	Chain	Res	Type
1	B	124	ASN
1	B	159	ASN
1	B	187	HIS
1	B	218	GLN
1	B	225	GLN
1	B	247	GLN
1	B	256	ASN
1	B	268	ASN
1	B	377	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FNS	B	9570	-	34,37,37	3.23	9 (26%)	42,58,58	2.34	9 (21%)
2	FNS	A	5570	-	34,37,37	3.54	10 (29%)	42,58,58	2.37	14 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FNS	B	9570	-	-	2/18/24/24	0/3/3/3
2	FNS	A	5570	-	-	2/18/24/24	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5570	FNS	O3S-S	13.67	1.65	1.42
2	B	9570	FNS	O3S-S	12.73	1.63	1.42
2	A	5570	FNS	O2S-S	11.51	1.61	1.42
2	B	9570	FNS	O2S-S	9.68	1.58	1.42
2	A	5570	FNS	C1'-N10	-6.38	1.32	1.48
2	B	9570	FNS	C1'-N10	-5.60	1.33	1.48
2	A	5570	FNS	C5'-C4'	-2.83	1.47	1.51
2	B	9570	FNS	C4'-C3'	-2.75	1.48	1.53
2	B	9570	FNS	C1'-C2'	-2.67	1.48	1.52
2	B	9570	FNS	C9-C8	-2.50	1.35	1.39
2	A	5570	FNS	C9-C9A	-2.46	1.35	1.39
2	A	5570	FNS	O1S-S	2.44	1.57	1.45
2	A	5570	FNS	C5A-N5	-2.36	1.33	1.41
2	A	5570	FNS	C1'-C2'	-2.31	1.49	1.52
2	A	5570	FNS	C2-N3	2.20	1.44	1.39
2	B	9570	FNS	C2-N1	2.17	1.41	1.36
2	B	9570	FNS	C5'-C4'	-2.15	1.48	1.51
2	B	9570	FNS	C9-C9A	-2.07	1.36	1.39
2	A	5570	FNS	C9-C8	-2.02	1.36	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	9570	FNS	O2S-S-O3S	-7.88	98.70	119.22
2	A	5570	FNS	O2S-S-O3S	-6.72	101.73	119.22
2	B	9570	FNS	C5'-C4'-C3'	-5.54	101.51	112.20
2	A	5570	FNS	C10-N1-C2	5.23	127.35	116.90
2	A	5570	FNS	C5'-C4'-C3'	-5.18	102.21	112.20
2	A	5570	FNS	C6-C5A-C9A	5.17	124.50	118.69
2	B	9570	FNS	C10-N1-C2	4.77	126.43	116.90
2	B	9570	FNS	N10-C10-N1	4.55	131.43	118.35
2	A	5570	FNS	N10-C10-N1	4.15	130.27	118.35
2	A	5570	FNS	O2-C2-N3	3.60	125.65	118.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	9570	FNS	C6-C5A-C9A	3.35	122.45	118.69
2	A	5570	FNS	O4'-C4'-C3'	3.09	116.60	109.10
2	A	5570	FNS	C5A-N5-C4A	2.98	126.77	120.47
2	B	9570	FNS	O3P-P-O5'	-2.98	98.80	106.73
2	B	9570	FNS	O4'-C4'-C3'	2.72	115.70	109.10
2	A	5570	FNS	C9-C8-C7	2.69	123.53	119.67
2	B	9570	FNS	C4-N3-C2	-2.57	120.89	125.64
2	B	9570	FNS	C5A-N5-C4A	2.43	125.60	120.47
2	A	5570	FNS	O3P-P-O5'	-2.27	100.69	106.73
2	A	5570	FNS	C4-N3-C2	-2.15	121.67	125.64
2	A	5570	FNS	O3'-C3'-C2'	2.14	113.97	108.81
2	A	5570	FNS	N3-C2-N1	-2.11	115.24	119.38
2	A	5570	FNS	C8M-C8-C9	-2.03	115.73	119.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5570	FNS	C5'-O5'-P-O1P
2	A	5570	FNS	C4'-C5'-O5'-P
2	B	9570	FNS	C4'-C5'-O5'-P
2	B	9570	FNS	C5'-O5'-P-O1P

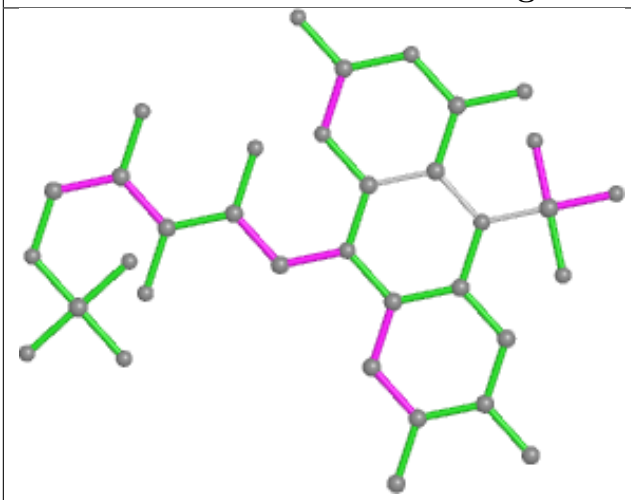
There are no ring outliers.

2 monomers are involved in 13 short contacts:

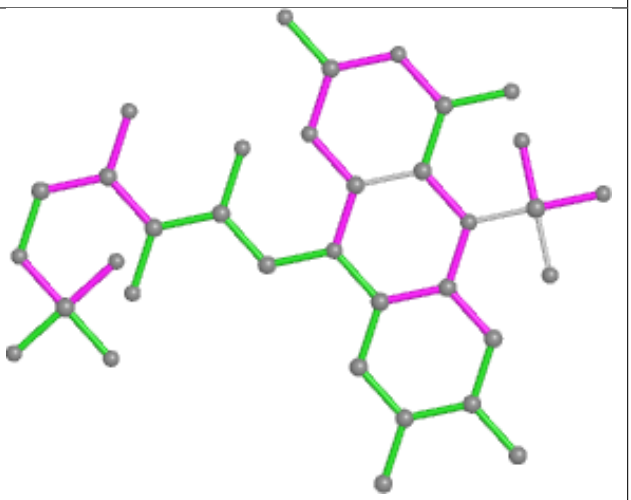
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	9570	FNS	11	0
2	A	5570	FNS	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

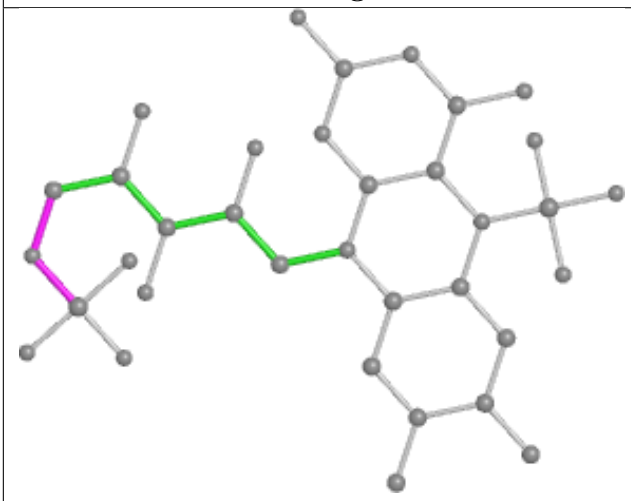
Ligand FNS B 9570



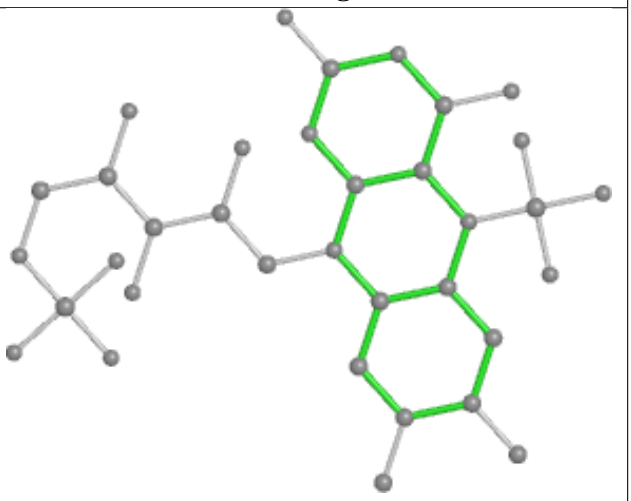
Bond lengths



Bond angles

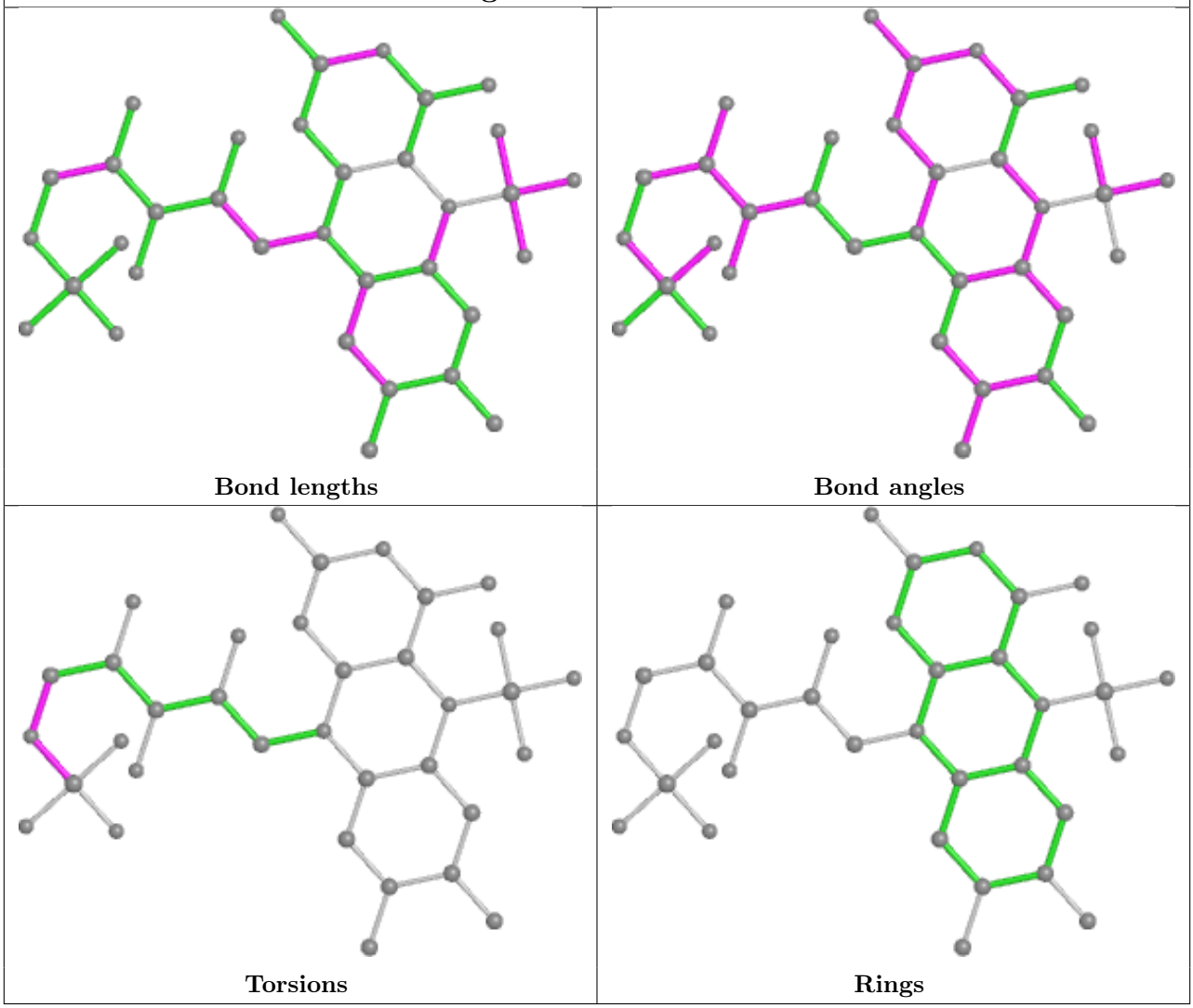


Torsions



Rings

Ligand FNS A 5570



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	392/511 (76%)	-0.13	20 (5%)	28	26	34, 48, 75, 85	0
1	B	387/511 (75%)	0.15	30 (7%)	13	11	36, 56, 84, 91	0
All	All	779/1022 (76%)	0.01	50 (6%)	19	18	34, 51, 81, 91	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	114	SER	7.7
1	A	300	THR	6.3
1	B	106	ILE	5.1
1	B	261	ILE	5.1
1	B	298	SER	5.0
1	A	106	ILE	4.8
1	A	511	ALA	4.6
1	A	114	SER	4.5
1	A	297	PHE	4.4
1	A	113	LYS	4.1
1	B	399	ASN	4.1
1	B	299	ASN	4.0
1	B	324	LYS	3.7
1	B	102	THR	3.5
1	B	103	LYS	3.4
1	A	103	LYS	3.4
1	B	245	ASP	3.3
1	B	240	GLU	3.2
1	A	102	THR	3.1
1	B	343	LYS	3.1
1	B	325	PHE	3.1
1	A	399	ASN	3.0
1	B	511	ALA	2.9
1	A	115	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	104	GLU	2.8
1	A	299	ASN	2.8
1	B	323	SER	2.7
1	B	105	ASP	2.7
1	A	298	SER	2.6
1	A	340	LYS	2.6
1	B	257	SER	2.6
1	B	260	LYS	2.6
1	B	243	PRO	2.6
1	B	246	LYS	2.6
1	A	101	GLU	2.5
1	B	113	LYS	2.5
1	B	206	LEU	2.5
1	A	175	ARG	2.5
1	B	258	ASP	2.4
1	A	105	ASP	2.4
1	B	107	ALA	2.4
1	A	271	LYS	2.4
1	A	397	GLN	2.3
1	B	397	GLN	2.3
1	B	110	GLU	2.2
1	B	104	GLU	2.2
1	A	343	LYS	2.1
1	B	194	VAL	2.1
1	B	279	VAL	2.1
1	B	295	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

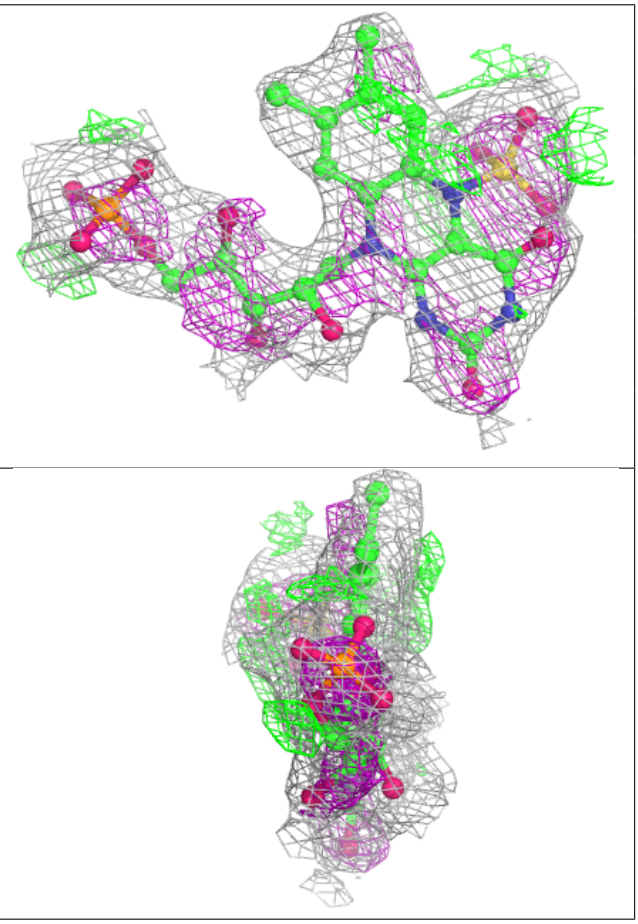
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FNS	A	5570	35/35	0.95	0.16	13,19,33,37	0
2	FNS	B	9570	35/35	0.95	0.20	15,21,32,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

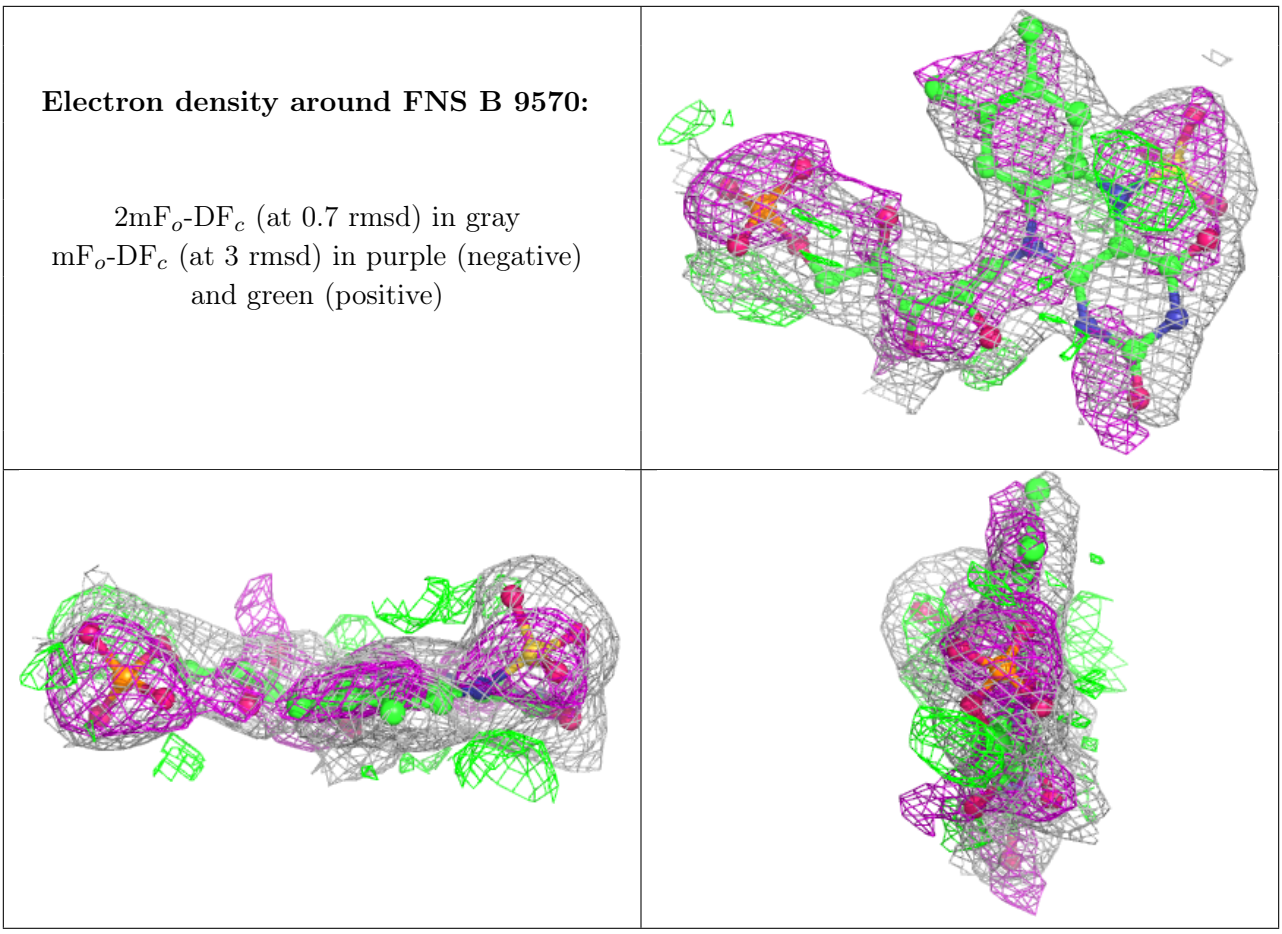
Electron density around FNS A 5570:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FNS B 9570:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.